

MAP 5485, Maple Tutorial 4

First open the worksheet in Maple tutorial 4. Use Maple to compute the following.

- (1) Let p_1, \dots, p_7 be the points given in the worksheet. These vectors give the coordinates of successive alpha carbons along the backbone of the protein *bacteriorhodopsin*. Find the distance matrix $(|p_i - p_j|^2)$ for these points for these points
- (2) Let $v_j = p_{j+1} - p_1$ for $j = 1, \dots, 6$. Find the Gram matrix $(v_i \cdot v_j)$.
- (3) Let G be the Gram matrix of the vectors v_1, v_2, v_3 . Diagonalize G (see below) by finding orthogonal matrix F and diagonal matrix D such that $FGF' = D$.
- (4) Note that the eigenvalues of G , the entries on the diagonal of D , are positive. Let \sqrt{D} be a matrix whose entries are the square roots of the entries in D . From the above we see that if $M = \sqrt{D}F$ then $M'M = G$. Find M and check that $M'M = G$.
- (5) Let $V = (v_1, v_2, v_3)$ be the matrix with columns v_1, v_2 and v_3 . Since G is the gram matrix of the vectors v_1, v_2, v_3 , we have that $V'V = G$. We have also shown that $M'M = G$ so that G is also the Gram matrix for the columns of M . Show that the two sets of vectors differ by a rotation, that is, there is a rotation matrix R such that $RV = M$. Find R .
- (6) Here is a case when there are only two distinct eigenvalues for a 3×3 matrix. Diagonalize the matrix

$$\begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}.$$

Note that if v_1 and v_2 are eigenvectors corresponding to the same eigenvalue λ then you can find an orthonormal set of eigenvectors v'_1 and v'_2 by setting

$$v'_1 = \frac{v_1}{|v_1|} \quad v'_2 = \frac{v_2 - (v'_1 \cdot v_2)v'_1}{|v_2 - (v'_1 \cdot v_2)v'_1|}$$

Diagonalization of symmetric matrices

To diagonalize an $n \times n$ symmetric matrix A .

- (1) Find an orthonormal set of eigenvectors, and create a column matrix F consisting of these eigenvectors. The eigenvectors and eigenvalues are always real for a symmetric matrix. Note that if there are n distinct eigenvalues then all the eigenvectors will be mutually perpendicular.
- (2) If there are less than n eigenvectors, then there will be more than one eigenvector corresponding to a given eigenvalue. You will need to convert these to an orthonormal set using the Gram-Schmidt procedure. If you are working numerically, Maple will usually return a normalized set of eigenvectors. But you should always check.

2

- (3) If D is a diagonal matrix consisting of the corresponding eigenvalues of A , then by definition of eigenvalues, $AF = FD$ and so $F'AF = D$ and A is diagonalized.